Connecting via Winsock to STN

Welcome to STN International! Enter x:x

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PASSWORD:
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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUL 02	LMEDLINE coverage updated
NEWS 3	JUL 02	SCISEARCH enhanced with complete author names
NEWS 4	JUL 02	CHEMCATS accession numbers revised
NEWS 5	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 6	JUL 16	CAplus enhanced with French and German abstracts
NEWS 7	JUL 18	CA/CAplus patent coverage enhanced
NEWS 8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9	JUL 30	USGENE now available on STN
NEWS 10	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 11	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 12	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 13	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 14	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 15	AUG 27	USPATOLD now available on STN
NEWS 16	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 17	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 18	SEP 13	FORIS renamed to SOFIS
NEWS 19	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS 20	SEP 17	CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 21	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS 22	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 23	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 24	OCT 19	BEILSTEIN updated with new compounds
NEWS 25	NOV 15	Derwent Indian patent publication number format enhanced
NEWS 26	NOV 19	WPIX enhanced with XML display format

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:11:43 ON 28 NOV 2007

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.15	3.15

FILE 'REGISTRY' ENTERED AT 17:20:56 ON 28 NOV 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 27 NOV 2007 HIGHEST RN 956075-61-9
DICTIONARY FILE UPDATES: 27 NOV 2007 HIGHEST RN 956075-61-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

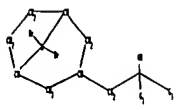
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

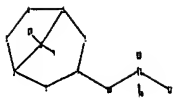
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10-565048genA.str





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chain nodes :
9  10  11  12  13  14  17
ring nodes :
1  2  3  4  5  6  7  8
chain bonds :
7-10  8-9  8-17  10-11  11-12  11-13  11-14
ring bonds :
1-2  1-7  2-3  2-8  3-4  4-5  5-6  5-8  6-7
exact/norm bonds :
1-2  1-7  2-3  2-8  3-4  4-5  5-6  5-8  6-7  11-12  11-13  11-14
exact bonds :
7-10  8-9  8-17  10-11


G1:Cb,Hy,Ak

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:CLASS  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  17:CLASS



L1       STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
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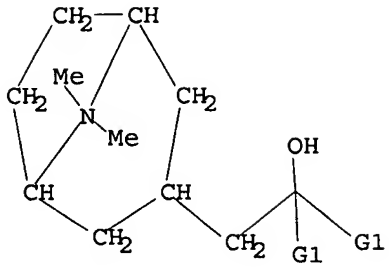

G1 Cb,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 17:21:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 165 TO ITERATE

100.0% PROCESSED 165 ITERATIONS 70 ANSWERS
SEARCH TIME: 00.00.01

L2 70 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	175.70

FILE 'CAPLUS' ENTERED AT 17:21:58 ON 28 NOV 2007
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FILE COVERS 1907 - 28 Nov 2007 VOL 147 ISS 23
FILE LAST UPDATED: 27 Nov 2007 (20071127/ED)

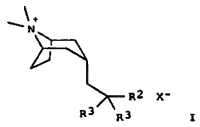
Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2
L3 7 L2

=> d l3 1-7 abs ibib hitstr

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
GI



I

AB Title compds. [I; R1, R2 = (substituted) Ph, thienyl, pyridyl, PhCH2, pyrimidinyl, thiazolyl, isothiazolyl, cycloalkyl, etc.; R3 = H, OH; X = physiol. acceptable anion], were prepared for treatment of chronic obstructive pulmonary disease, chronic bronchitis, asthma, chronic respiratory obstruction, pulmonary fibrosis, emphysema, and allergic rhinitis (no data). Thus, 2-[(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]-1,1-bis(3-methyl-2-thienyl)ethanol (preparation given) was treated with MeBr in tert-Bu Me ether to give 61% (3-endo)-3-[2-hydroxy-2,2-bis(3-methyl-2-thienyl)ethyl]-8,8-dimethyl-8-azoniabicyclo[3.2.1]octane bromide.

ACCESSION NUMBER: 2007:146107 CAPLUS
DOCUMENT NUMBER: 146:229203
TITLE: Preparation of azoniabicyclooctanes as M3 muscarinic acetylcholine receptor antagonists.
INVENTOR(S): Busch-Petersen, Jakob; Laine, Dramane Ibrahim; Palovich, Michael R.; Davis, Roderick S.; Fu, Wei; Xie, Haibo
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 42pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007016639	A2	20070208	WO 2006-US30153	20060802
WO 2007016639	A3	20070705		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-704579P P 20050802

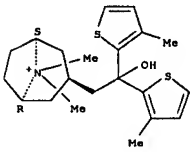
OTHER SOURCE(S): MARPAT 146:229203

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 924646-68-4P 924646-70-8P 924646-72-0P
924646-74-2P 924646-76-4P 924646-78-6P
924655-67-4P 924655-70-9P 924655-72-1P
924655-73-2P 924655-75-4P 924655-77-6P
924655-78-7P 924655-80-1P 924655-81-2P
924655-82-3P 924655-83-4P 924655-84-5P
924655-85-6P 924655-89-0P 924655-90-3P
924655-91-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of azoniabicyclooctanes as M3 muscarinic acetylcholine receptor antagonists)

RN 924646-68-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(3-methyl-2-thienyl)ethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

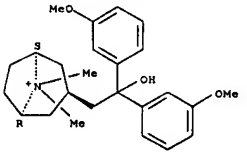
Relative stereochemistry.



● Br⁻

RN 924646-70-8 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(3-methoxyphenyl)ethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.

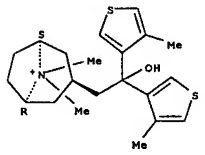


● I⁻

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 924646-72-0 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(4-methyl-3-thienyl)ethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

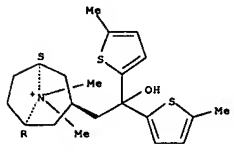
Relative stereochemistry.



● Br⁻

RN 924646-74-2 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(5-methyl-2-thienyl)ethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.

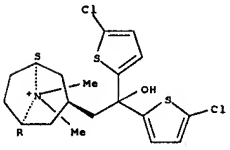


● Br⁻

RN 924646-76-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(5-chloro-2-thienyl)-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.

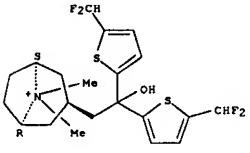
L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

RN 924646-78-6 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis[5-(difluoromethyl)-2-thienyl]-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

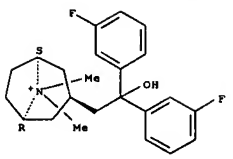
Relative stereochemistry.



● Br⁻

RN 924655-67-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(3-fluorophenyl)-2-hydroxyethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

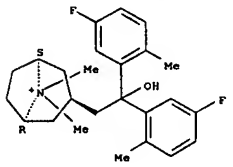
Relative stereochemistry.



● I^-

RN 924655-70-9 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(5-fluoro-2-methylphenyl)-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

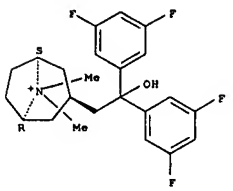
Relative stereochemistry.



● Br^-

RN 924655-72-1 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-hydroxy-2,2-di-3-thienylethyl)-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

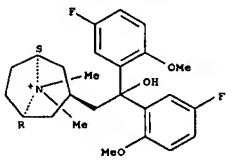
Relative stereochemistry.



● Br^-

RN 924655-77-6 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(5-fluoro-2-methoxyphenyl)-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

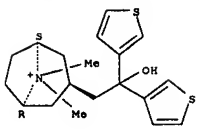
Relative stereochemistry.



● Br^-

RN 924655-78-7 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(3-fluoro-2-methylphenyl)-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

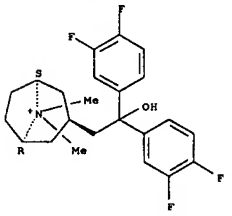
Relative stereochemistry.



● I^-

RN 924655-73-2 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(3,4-difluorophenyl)-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

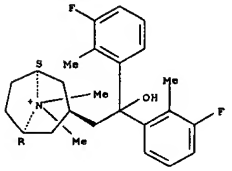
Relative stereochemistry.



● Br^-

RN 924655-75-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(3,5-difluorophenyl)-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

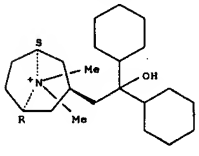
Relative stereochemistry.



● Br^-

RN 924655-80-1 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(2,2-dicyclohexyl-2-hydroxyethyl)-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

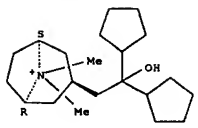
Relative stereochemistry.



● Br^-

RN 924655-81-2 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(2,2-dicyclopentyl-2-hydroxyethyl)-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

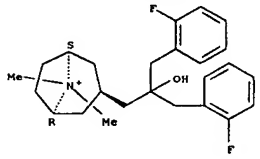
Relative stereochemistry.



● Br^-

RN 924655-82-3 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[3-(2-fluorophenyl)-2-[(2-fluorophenyl)methyl]-2-hydroxypropyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

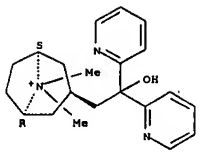
Relative stereochemistry.



● Br^-

RN 924655-83-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-hydroxy-2,2-di-2-pyridinylethyl)-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

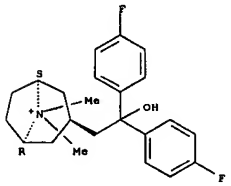
Relative stereochemistry.



● I^-

RN 924655-84-5 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(4-fluorophenyl)-2-hydroxyethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

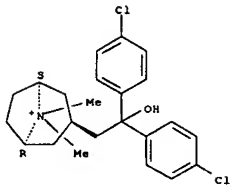
Relative stereochemistry.



● I^-

RN 924655-85-6 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(4-chlorophenyl)-2-hydroxyethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

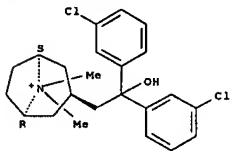
Relative stereochemistry.



● I^-

RN 924655-89-0 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(3-chlorophenyl)-2-hydroxyethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

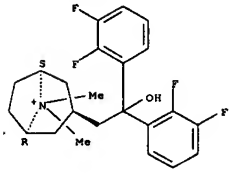
Relative stereochemistry.



● I^-

RN 924655-90-3 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(2,2-bis(2,3-difluorophenyl)-2-hydroxyethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

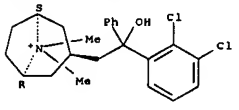
Relative stereochemistry.



● I^-

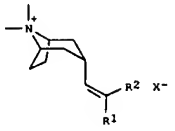
RN 924655-91-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-(2,3-dichlorophenyl)-2-hydroxy-2-phenylethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



● I^-

L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
GI



I

AB Title compds. [I; R1, R2 = (substituted) Ph, thienyl, pyridyl, PhCH2, pyrimidinyl, thiazolyl, isothiazolyl, cycloalkyl, etc.; X = pharmaceutically acceptable counterion], were prepared for treatment of COPD, chronic bronchitis, asthma, chronic respiratory obstruction, pulmonary fibrosis, emphysema, and allergic rhinitis (no data). Thus, (endo)-3-[2,2-bis(3-hydroxyphenyl)ethenyl]-8,8-dimethyl-8-azoniabicyclo[3.2.1]octane bromide was prepared from tri-Me phosphonoacetate, tropinone, MeI, and 3-methoxyphenylmagnesium bromide.

ACCESSION NUMBER: 2007:144089 CAPLUS
DOCUMENT NUMBER: 146:229182
TITLE: Preparation of 3-(arylethenyl)-8,8-dimethyl-8-azoniabicyclo[3.3.1]octanes as M3 muscarinic acetylcholine receptor antagonists.
INVENTOR(S): Busch-Petersen, Jakob; Laine, Dramane Ibrahim; Palovich, Michael R.; Davis, Roderick S.; Fu, Wei; Xie, Haibo
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 35pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007016650	A2	20070208	WO 2006-US30218	20060802
WO 2007016650	A3	20070531		

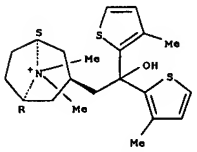
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-704578P P 20050802

OTHER SOURCE(S): MARPAT 146:229182

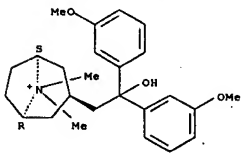
L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

RN 924646-70-8 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(3-methoxyphenyl)ethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



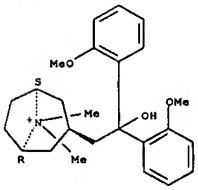
● I⁻

RN 924646-72-0 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(4-methyl-3-thienyl)ethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.

L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 924646-91-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylethenyldimethylazoniabicyclooctanes as M3 muscarinic
acetylcholine receptor antagonists)
RN 924646-91-3 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(2-methoxyphenyl)ethyl]-8,8-dimethyl-, iodide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.

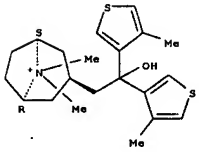


● I⁻

IT 924646-68-4P 924646-70-8P 924646-72-0P
924646-74-2P 924646-76-4P 924646-78-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylethenyldimethylazoniabicyclooctanes as M3 muscarinic
acetylcholine receptor antagonists)
RN 924646-68-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(3-methyl-2-thienyl)ethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.

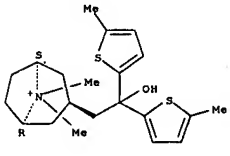
L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

RN 924646-74-2 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2,2-bis(5-methyl-2-thienyl)ethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.

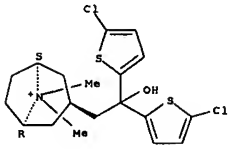


● Br⁻

RN 924646-76-4 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis(5-chloro-2-thienyl)-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.

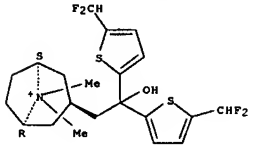
L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br⁻

RN 924646-78-6 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2,2-bis[5-(difluoromethyl)-2-thienyl]-2-hydroxyethyl]-8,8-dimethyl-, bromide (1:1), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



● Br⁻

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
AB Muscarinic acetylcholine receptor antagonists, e.g., (3-endo)-3-(2-hydroxy-2,2-diphenylethyl)-8,8-dimethyl-8-azoniabicyclo[3.2.1]octane bromide and methods of using them are provided. In addition a pharmaceutical composition for the treatment of muscarinic acetylcholinereceptor-mediated diseases comprising the above compound is disclosed.

ACCESSION NUMBER: 2005:99316 CAPLUS
DOCUMENT NUMBER: 142:183475
TITLE: Muscarinic acetylcholine receptor antagonists
INVENTOR(S): Belmonte, Kristen E.; Busch-Petersen, Jakob; Laine, Dramane; Palovich, Michael R.
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

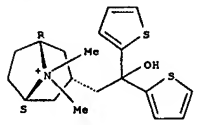
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005009362	A2	20050203	WO 2004-US23041	20040716
WO 2005009362	A3	20050407		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004259238	A1	20050203	AU 2004-259238	20040716
CA 2532433	A1	20050203	CA 2004-2532433	20040716
EP 1648461	A2	20060426	EP 2004-778509	20040716
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1822839	A	20060823	CN 2004-80020652	20040716
BR 2004012537	A	20060919	BR 2004-12537	20040716
JP 2007525478	T	20070906	JP 2006-520387	20040716
IN 2006DN00077	A	20070824	IN 2006-DN77	20060104
MX 2006PA00663	A	20060330	MX 2006-PA663	20060117
US 2006178396	A1	20060810	US 2006-565048	20060117
NO 2006000777	A	20060411	NO 2006-777	20060217

PRIORITY APPLN. INFO.:			US 2003-487982P	P 20030717
			WO 2004-US23041	W 20040716

OTHER SOURCE(S): MARPAT 142:183475
IT 90114-71-9 102133-77-7 106655-98-5
106713-93-3 106954-22-7 834882-84-7
834882-85-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(muscarinic acetylcholine receptor antagonists)
RN 90114-71-9 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-hydroxy-2,2-di-2-thienylethyl)-8,8-

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

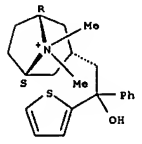
Relative stereochemistry.



● Br⁻

RN 102133-77-7 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2-phenyl-2-(2-thienyl)ethyl]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

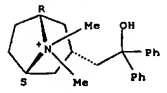
Relative stereochemistry.



● Br⁻

RN 106655-98-5 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane,
3-(2-hydroxy-2,2-diphenylethyl)-8,8-dimethyl-
, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

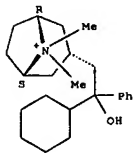


● Br⁻

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 106713-93-3 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane,
3-(2-cyclohexyl-2-hydroxy-2-phenylethyl)-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

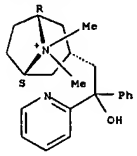
Relative stereochemistry.



● Br⁻

RN 106954-22-7 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane,
3-[2-hydroxy-2-phenyl-2-(2-pyridinyl)ethyl]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

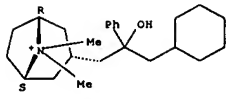


● Br⁻

RN 834882-84-7 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(3-cyclohexyl-2-hydroxy-2-phenylpropyl)-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



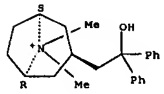
● Br⁻

RN 834882-85-8 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane,
3-(2-hydroxy-2,2-diphenylethyl)-8,8-dimethyl-
, (3-endo)-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA
INDEX
NAME)

CM 1

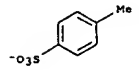
CRN 805224-99-1
CMF C23 H30 N O

Relative stereochemistry.



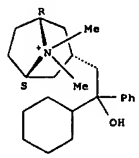
CM 2

CRN 16722-51-3
CMF C7 H7 O3 S



L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
0.1-1.0; VI, α, 1, 2-cyclohexylethyl, Ph,--,--,--,--, HCl
198-200°. --; VI, α, 1, Ph, 2-pyridyl,--,--,--,--, tartrate
78-80°picrate 201-3°, --; and VI, α, 2, Ph,
Ph,--,--,--,--, citrate 170°, MeBr 277°, citrate
0.001-0.010, MeBr salt 0.01.
ACCESSION NUMBER: 1963:27160 CAPLUS
DOCUMENT NUMBER: 58:27160
ORIGINAL REFERENCE NO.: 58:4510b-h
TITLE: 3-Substituted tropane derivatives. III. 3-Substituted tropane carbinols, alkenes, and alkanes
AUTHOR(S): Zirkle, Charles L.; Anderson, Elvin L.; Craig, Paul N.; Gerns, Fred R.; Indik, Zena K.; Pavloff, Alex M.
CORPORATE SOURCE: Smith, Kline, & French Labs., Philadelphia, PA
SOURCE: Journal of Medicinal & Pharmaceutical Chemistry (1962), 5, 341-56
CODEN: JMPCAS; ISSN: 0095-9065
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:27160
IT 106713-93-3
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 106713-93-3 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane,
3-(2-cyclohexyl-2-hydroxy-2-phenylethyl)-8,8-
dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

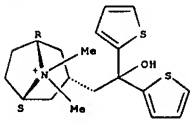


● Br⁻

IT 90114-71-9P, 8-Azoniabicyclo[3.2.1]octane, 3-(2-hydroxy-2,2-di-2-thienylethyl)-8,8-dimethyl-, bromide 102133-77-7P, 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2-phenyl-2-(2-thienyl)ethyl]-8,8-dimethyl-, bromide 106655-98-5P, 8-Azoniabicyclo[3.2.1]octane,
3-(2-hydroxy-2,2-diphenylethyl)-8,8-dimethyl-,
bromide 106954-22-7P, 8-Azoniabicyclo[3.2.1]octane,
3-[2-hydroxy-2-phenyl-2-(2-pyridinyl)ethyl]-8,8-dimethyl-, bromide
RL: PREP (Preparation)
(preparation of)
RN 90114-71-9 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-hydroxy-2,2-di-2-thienylethyl)-8,8-
dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
GI For diagram(s), see printed CA Issue.
AB cf. CA 57, 3389b. For testing as cholinolyti: agents, a series of 3-substituted tropane derivs. (Ia) were prepared by the following sequence:
(X = 3α-, or 3β-tropinyl) X(CH2)nCO2Me → X(CH2)nCOR (I)
→ X(CH2)nC(OH)RR' (II) → X: CRR' (III), XCH:CRR' (IV), or
XCH2CH:CRR' (V) → X(CH2)nCHRR' (VI) using the procedures followed by Adamson for open-chain analogs (Adamson, et al., CA 45, 8462f). Compds. prepared were (compound number, tropinyl group configuration, n, R, R', %
yield, m.p., b.p./pressure, n25D, salts prepared with m.p. of each, and relative activity (atropine = 1) given): I, α, 0, 2-thienyl, --, 4.4, --, 142-3°/ 0.4, --; picrate 259°, --; I, α, 1, Ph, --, 75,--, 140-3°/0.2,--, HCl 140-3°, --; I, α, 1, cyclohexyl, --, 35, --, 142-4°/0.8, --, picrate 165-8°, MeBr 297-9°, --; I, α, 1, 2-cyclohexylethyl, --, 74, --, 157-64°/0.7, 1.5010, picrate 148-50°, --; I, α, 2, Et, --, 77, --, 105-9°/0.35, 1.4870, picrate 123.0-4.5°, --; II, β, O, Me, Me, 84, --, 116-19°/4, --, picrate 167.5-9.0°, MeI 199-202°, --; II, α, O, 2-thienyl, 2-thienyl, 8.0, 157.5-9.0°,--,--,--,--; II, α, O, Ph, Ph, 47, 185.5-6.0°, --, --, HCl 290°, citrate 112-18% picrate 214.0-15.5°, MeBr 309-10°, citrate 0.001, MeBr salt 0.1; II, β, O, Ph, Ph, 86, 182-4°,--,--, HCl 325°, picrate 230-1°, HCl salt 0.001; II, α, 1, Ph, Ph, 76, 147-8°, --, --, HCl 235°, HBr 230°, MeBr 282°, HCl salt 1, MeBr salt 0.1-1.0; II, β, 1, Ph, Ph, --, 178-9°, --, --, HCl 253.5°, HCl salt 0.001; II, α, 1, cyclohexyl, Ph, 90, 139.0-40.5°,--,--, HCl 254-5°, MeBr 262°, HCl salt 0.1; II, α, 1, 2-cyclohexylethyl, Ph, above 66, 104-6°,--,--, HCl 215-16°, citrate 134-6°, MeBr 263-5°, HCl salt 0.01; II, α, 1, Ph, Et, 12, --, --, --, HCl 237°, HCl salt 0.01-0.10; II, α, 1, 2-pyridyl, Ph, 64, 117.5-18.5°, --, --, HI 194-6°, dipicrate 191-2°, MeBr 268°, HI salt 0.01; II, α, 1, Ph, 2-thienyl, 73, 137.5-9.0°,--,--, maleate 145-6°, MeBr 256°, maleate 1; II, α, 1,2-thienyl, 2-thienyl, 69, 138-40°, --, --, HOAc 189-90°, MeBr 245.5°, HOAc salt 1; II, α, 2, Ph, Ph, 92, 142-3°, --, --, HCl 249-50°, MeBr 299°, HCl salt 0.01, MeBr salt 0.1; III, --, --, Ph, Ph,--,--,--,--,--,HCl 275-8°, picrate 237-8°, MeBr 281-5°, HCl salt 0.01, MeBr salt 0.1-1.0; III,--,--, 2-thienyl, 2-thienyl, 76 --,--,-- HCl 224-5°, --; IV, α, --, Ph, Ph, 100, 111-12°, --, --, HCl 217-18°, picrate 186-8°, MeBr 286° HCl salt 1-10, MeBr salt 0.1-1.0; IV, α --, cyclohexyl, Ph, 95,--,--,--,--, HCl 195-6°, HI 222.5-4.0°, MeBr 250-5° HCl salt 1; IV, α, --, Ph, Et,--,--,--,--,--, HCl 214-15°, --; IV, α, --, Ph, 2-pyridyl, 78, 97.5-9.5, --, -- tartrate 165-7°, picrate 204-6°, MeBr 227-8°, --; IV, α, --, Ph, 2-thienyl, 96, 65-70, --, --, HCl 194-200° tartrate 174-5° picrate 209-10°, MeBr 258-9°, tartrate 0.1-1.0; IV, α, --, 2-thienyl, 2-thienyl, 76,--,--,--, HCl 230-2°,picrate 190-2°, MeBr 252-3°, HCl salt 1; V, α, --, Ph, Ph, --,--,--, citrate 174°, MeBr 280°, citrate 0.001, MeBr salt 0.01; VI, α, O, Me, Me, -- --, 109-11°/29, 1.4739, HCl 194- 6% MeI 224-6°,--; VI, α, O, Ph, Ph,--, 70-2°,--,--, HCl above 310°, MeBr 277-8°, HCl 0.01, MeBr salt 0.1; VI, α, 1,Ph, Ph,--,--,--,--, HCl 244-5°, MeBr 257-8° HCl salt 1-10, MeBr 1; VI, α, 1, cyclohexyl, Ph,--,--,--,--, HCl 167.0-8.5°, citrate 153-5°, picrate 140-1°, MeBr 259-60°, citrate

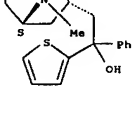
L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Relative stereochemistry.



● Br⁻

RN 102133-77-7 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane, 3-[2-hydroxy-2-phenyl-2-(2-thienyl)ethyl]-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

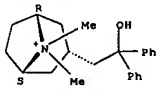
Relative stereochemistry.



● Br⁻

RN 106655-98-5 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane,
3-(2-hydroxy-2,2-diphenylethyl)-8,8-dimethyl-
, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

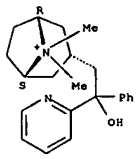


● Br⁻

RN 106954-22-7 CAPLUS

L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 8-Azoniabicyclo[3.2.1]octane,
3-[2-hydroxy-2-phenyl-2-(2-pyridinyl)ethyl]-
8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

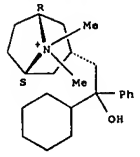
Relative stereochemistry.



● Br⁻

L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
AB It had been known that, as by-products in the synthesis of 2-methyl-5-ethylpyridine by the condensation of paraldehyde with NH3, α-picoline, γ-picoline, 3-ethyl-4-methylpyridine, 2-methyl-5-(trans-2-butenyl)pyridine, 2-(trans-propenyl)-5-ethylpyridine, 2-methyl-5-(trans-1-butenyl)pyridine (I), 2-methyl-5-(3-aminobutyl)pyridine, 2-methyl-3-ethylpyridine (II), and 2,6-dimethyl-3-ethylpyridine were formed. In the author's expts., I and II were not found, but in addition to the above compds., the existence of 2-propyl-5-ethylpyridine, 2-methyl-5-butylpyridine, 2-methyl-5-(cis-1-butenyl)pyridine, 2-(cis-propenyl)-5-ethylpyridine, and N-ethylacetamide was confirmed, along with an unknown high-boiling C5H5N derivative having a secondary amino group in the side chain. The amount of each by-product was determined by gas chromatography, and the mechanism of their formation was discussed.
ACCESSION NUMBER: 1963:27159 CAPLUS
DOCUMENT NUMBER: 58:27159
ORIGINAL REFERENCE NO.: 58:4509h,4510a-b
TITLE: By-products formed in the manufacture of 2-methyl-5-ethylpyridine
AUTHOR(S): Motoda, Tsuneo; Omae, Tsutomu; Yamamoto, Hiroshi; Yoshie, Yoichi
CORPORATE SOURCE: Nippon Synthetic Chemical Industry Co., Ltd., Amagasaki
SOURCE: Kogyo Kagaku Zasshi (1962), 65, 354-9
CODEN: KGKZA7; ISSN: 0368-5462
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 106713-93-3
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 106713-93-3 CAPLUS
CN 8-Azoniabicyclo[3.2.1]octane,
3-(2-cyclohexyl-2-hydroxy-2-phenylethyl)-8,8-dimethyl-, bromide, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



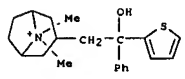
● Br⁻

L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN
AB Me 3-tropanecarboxylate (10.1 g.) in 100 ml. Et2O stirred 1.5 hrs. at room temperature with PhLi gave diphenyl-3-tropanylcarbinol, m. 214-15° (aqueous MeOH); citrate, m. 112-18° (iso-PrOH-Et2O); methobromide, m. 309-10° (alc.). Et 3-tropaneacetate (I) (10 g.) in 20 ml. Et2O refluxed with PhLi and 11.8 g. thiophene in Et2O gave 1,1-di(2-thienyl 3-tropaneethanol, m. 138-40° (EtOAc); acetate, m. 189-90°; methobromide, m. 245.5° (alc.). 1,1-Diphenyl-3-tropaneethanol-HCl, m. 234-5° (alc.-Et2O); methobromide, m. 282-3° (alc.-Et2O). I with concentrated HCl gave 3-tropaneacetic acid-HCl (II), m. 172-4°. II (11 g.) refluxed with PhLi gave Ph 3-tropanylmethyl ketone (III), b0.2 138-41°. III (9 g.) stirred several hrs. at room temperature with PhLi gave 1,1-diphenyl-3-tropaneethanol-HBr, m. 230°. III (10 g.) treated with PhLi and thiophene gave 1-phenyl-1-(2-thienyl)-3-tropaneethanol, m. 137.5-9.0°; maleate, m. 145-6° (alc.-Et2O); methobromide, m. 256° (alc.). 1-Phenyl-1-(2-pyridyl)-3-tropaneethanol-HI, m. 194-6°; methobromide, m. 268° (alc.). 1-Ethyl-1-phenyl-3-tropaneethanol-HCl, m. 237-7.5° (alc.). 1-Cyclohexyl-1-phenyl-3-tropaneethanol-HCl, m. 254-5° (alc.-Et2O); methobromide, m. 262° (alc.-Et2O). 2-Cyclohexylethyl 3-tropanylmethyl ketone picrate, m. 148-50°; 1-(2-cyclohexylethyl)-1-phenyl-3-tropaneethanol-HCl, m. 215-16°; citrate, m. 134-6° (Me2CO-MeOH); methobromide, m. 263-5°. II (3.7 g.) treated with SOCl2 gave the acid chloride HCl salt which treated with CH2N2 gave the diazomethyl 3-tropanylmethyl ketone and subsequent treatment with Ag2O oxide gave Et 3-tropanepropionate (IV). IV (18 g.) treated with PhLi as above gave 1,1-diphenyl-3-tropanepropanol, m. 141-2.5°; HCl salt, m. 249-50°; methobromide salt, m. 299°. Cyclopentyl 3-(3-tropanyl)propyl ketone (6.6 g.) treated with PhLi as above gave 1-cyclopentyl-1-phenyl-3-tropanebutanol. Diphenyl-3-tropanecarbinol etho(ethyl sulfate) was a white solid. 1,1-Diphenyl-3-tropaneethanol metho-p-toluenesulfonate, m. 172-4°; etho(ethyl sulfate), m. 234-5°; butobromide, m. 225-7°; butiodide, m. 227-9°. 1-Cyclohexyl-1-phenyl-2-(3-tropane)ethanol butyl bromide was a white solid.
ACCESSION NUMBER: 1958:93023 CAPLUS
DOCUMENT NUMBER: 52:93023
ORIGINAL REFERENCE NO.: 52:16401g-i,16402a-b
TITLE: 8-Alkylnortropane derivatives
INVENTOR(S): Zirkle, Charles L.
PATENT ASSIGNEE(S): Smith, Kline & French Laboratories
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2800481		19570723	US 1955-519649	19550701

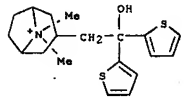
IT 112717-86-9P, 3-(β-Hydroxy-β-2-thienylphenethyl)-8-methyltropanium bromide 113222-63-2P, 3-(2-Hydroxy-2,2-di-2-thienylethyl)-8-methyltropanium bromide 114863-60-4P, 3-(β-Cyclohexyl-β-hydroxyphenethyl)-8-methyltropanium bromide 119016-27-2P, 3-(4-Cyclohexyl-2-hydroxy-2-phenylbutyl)-8-methyltropanium bromide
RL: PREP (Preparation)
(preparation of)
RN 112717-86-9 CAPLUS
CN 3-(β-Hydroxy-β-2-thienylphenethyl)-8-methyltropanium bromide

L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(6CI) (CA INDEX NAME)



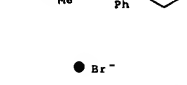
● Br⁻

RN 113222-63-2 CAPLUS
CN 3-(2-Hydroxy-2,2-di-2-thienylethyl)-8-methyltropanium bromide (6CI) (CA INDEX NAME)



● Br⁻

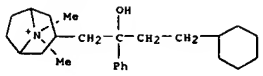
RN 114863-60-4 CAPLUS
CN 3-(β-Cyclohexyl-β-hydroxyphenethyl)-8-methyltropanium bromide (6CI) (CA INDEX NAME)



● Br⁻

RN 119016-27-2 CAPLUS
CN 3-(4-Cyclohexyl-2-hydroxy-2-phenylbutyl)-8-methyltropanium bromide (6CI) (CA INDEX NAME)

L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● Br^-

L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

AB Some new physiologically active 3-substituted-8-alkylnortropanes, the nontoxic organic and inorg. salts, and the quaternary ammonium salts are described. Me 3-(3-hydroxytropane)carboxylate (10 g.) in 50 ml. Ac2O heated 4 hrs. at 100°, the excess Ac2O and AcOH removed in vacuo, the residue poured into H2O, extracted with Et2O, and the Et2O evaporated gave Me 3-(3-acetoxytropane)-carboxylate (I), m. 66-7°, b15 162-5°. I (29 g.) added dropwise during 7 min. to a vertical tube heated to 420° and filled with pieces of Pyrex tubing, the apparatus swept with N, the product dissolved in dilute HCl, extracted with Et2O, the aqueous acid solution saturated with K2CO3, and the product separated gave Me 3-(2-tropene)carboxylate (II), b15 131-4°, n25.5D 1.4998. II (13 g.) in 100 ml. MeOH hydrogenated over 5 g. Raney Ni at 50 lb./sq. in. at room temperature and the mixture distilled gave Me 3-tropanecarboxylate (III), b18 128-32°, n25D 1.4819. III (10.1 g.) in 100 ml. Et2O stirred 1.5 hrs. at room temperature with a solution of PhLi (from 34.5 g. PhBr and 3.5 g. Li) in 100 ml. Et2O, the mixture added to 150 ml. H2O, and the solid collected and purified gave diphenyl-3-tropanecarbinol (IV), m. 185.5-6.0° (EtOAc). IV (5.6 g.) in 20 ml. AcOH and 25 ml. dilute HCl refluxed 10 min. and evaporated to dryness gave 3-benzhydrylidenetropane-HCl, m. 275-8° (alc.-Et2O); free base (V), a colorless oil. V (4 g.) in alc. hydrogenated over Raney Ni at 400 lb./sq. in. at 60° and the product chromatographed on Al2O3 gave 3-benzhydryltropane (VI), m. 70-2°. VI (1 g.) gave the HCl salt, unmelted below 310°; MeBr salt, m. 277-9°; etho(ethyl sulfate), white solid. Tropinone (13.9 g.), 11.3 g. NCCH2CO2Et, 1.6 g. NH4OAc, 7.3 g. AcOH, 20 ml. alc., and 0.6 g. Pd-C shaken under H at 50° and 60 lb./sq. in. gave Et α-cyano-3-tropaneacetate (VII), b0.3 116-18°, n24D 1.4942. VII (8 g.) in 30 ml. 37% HCl refluxed 13 hrs. and the crude 3-tropaneacetic acid-HCl esterified by leaving 3 days at room temperature in 50 ml. alc. with dry HCl gave Et 3-tropaneacetate (VIII), b2 104-5°, n25D 1.4774. VIII (42 g.) in 100 ml. Et2O similarly treated with PhLi gave 1,1-diphenyl-3-tropaneethanol (IX), m. 146.5-7.5° (EtOAc). IX (14.6 g.) in 29 ml. 37% HCl and 100 ml. AcOH refluxed 0.5 hr. gave 1,1-diphenyl-2-(3-tropanyl)ethylene (X), as the HCl salt, m. 217-18° (alc.-Et2O); free X, m. 109.5-10.0° (Me2CO). X (10 g.) in alc. hydrogenated over Raney Ni at 500 lb./sq. in. and 60° gave 1,1-diphenyl-2-(3-tropanyl)ethane, colorless oil; HCl salt, m. 244-5°; methobromide, m. 257-8° (alc.-Et2O); metho-p-toluenesulfonate, white solid; maleate, obtained by treating with maleic acid in alc. VIII in 37% HCl refluxed several hrs. gave 3-tropaneacetic acid-HCl (XI), m. 172-4° (MeOH-Et2O). XI (11 g.) similarly treated with PhLi followed by passage of HCl gave the HCl salt which when washed was reconverted to phenyl 3-tropanylmethyl ketone (XII), b0.2 138-41°. BuLi (from 3.7 g. BuCl and 0.7 g. Li) in 25 ml. Et2O treated slowly at -45° with 5.5 g. 2-bromopyridine in 10 ml. Et2O, the mixture stirred 10 min., and 2.5 g. XII in 30 ml. Et2O added slowly, the mixture stirred 15 min. at -15°, 50 ml. H2O added, the mixture stirred a further 15 min., a solid collected, the solid stirred with CHCl3 and H2O, and the CHCl3 layer removed, combined with the Et2O layer and evaporated gave 1-phenyl-1-(2-pyridyl)-3-tropaneethanol (XIII), m. 117-18.5°

L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(EtOAc). XIII (1 g.) and 2 ml. 85% H2SO4 heated 15 min. at 155° and the soln. made basic gave 1-phenyl-1-(2-pyridyl)-2-(3-tropanyl)ethylene (XIV), m. 97.5-9.5° (Me2CO). XIV (0.2 g.), 5 g. cyclohexane, and 0.3 g. 20% Pd-C refluxed 48 hrs. gave 1-phenyl-1-(2-pyridyl)-2-(3-tropanyl)ethane (XV) as a thick oil; picrate, m. 201-3° (aq. Me2CO). XV also forms the tartrate, m. 78-80° (alc.-Et2O). XII (12.2 g.) in 50 ml. Et2O added slowly to EtMgBr soln. (from 7.3 g. Mg) at 0°, the mixt. stirred 1.5 hrs. at room temp., then refluxed 1.5 hrs., decompd. with ice and 21 g. NH4Cl in 50 ml. H2O, the Et2O layer removed, and the aq. phase extd. with CHCl3 gave 1-ethyl-1-phenyl-3-tropaneethanol (XVI), m. 119-20°. XVI (0.44 g.) was dehydrated by heating 40 min. at 100° with 3 ml. concd. HCl to the ethylene, m. 170-200°. The ethylene hydrogenated in alc. over Raney Ni at 60° and 500 lb./sq. in. gave 1-ethyl-1-phenyl-2-(3-tropanyl)ethane (XVII), an oil, which formed an HCl salt. VIII (15 g.) similarly treated with 2-cyclohexylethylmagnesium bromide gave 2-cyclohexylethyl 3-tropanylmethyl ketone (XVIII), b0.7 157-64°, n24.5D 1.5010. XVIII (7.7 g.) in 20 ml. Et2O similarly treated with PhLi (from 9.5 g. PhBr) in Et2O at 0° gave 1-(2-cyclohexylethyl)-1-phenyl-3-tropaneethanol (XIX), m. 104-6° (EtOAc). XIX (0.5 g.), 1 ml. HI, 3 ml. AcOH, and 0.13 g. red P refluxed 3.5 hrs., the soln. filtered, the filtrate dild. with H2O, the crude HI salt sepd. as an oil and crystd. gave 1-(2-cyclohexylethyl)-1-phenyl-2-(3-tropanyl)ethane-HI, m. 175° (alc.-Et2O). The free base was a colorless oil; HCl salt, m. 198-200°. Similarly, 25 g. VIII reacted with cyclohexylmagneaium bromide to give cyclohexyl 3-tropanylmethyl ketone (XX), b0.9-1.1 142-53°, crystg. to a white solid on standing. XX (10 g.) similarly treated with PhLi gave 1-cyclohexyl-1-phenyl-3-tropaneethanol (XXI), m. 139-40.5° (EtOAc). XXI (1 g.) refluxed 0.5 hr. with AcOH and concd. HCl gave the ethylene HCl salt, m. 195-6°. Hydrolysis gave the free base as an oil. The free base (4.4 g.) hydrogenated over Raney Ni at 500 lb./sq. in. and 60° gave 1-cyclohexyl-1-phenyl-2-(3 tropanyl)ethane, colorless oil; HCl salt, m. 167-8.5°; citrate, m. 153-5°; butiodide, white solid. N-Isopropylnortropanone (16.7 g.), 11.3 g. NCCH2CO2Et, 1.6 g. NH4OAc, 7.3 g. AcOH, 20 ml. alc., and 0.6 g. Pd-C shaken with H at 60 lb./aq. in. and 60°, the residue refluxed 12 hrs. with concd. HCl gave crude 3-(N-isopropylnortropane)-acetic acid-HCl which was esterified with anhyd. MeOH and HCl 3 days at room temp. gave Me 3-(N-isopropylnortropane)acetate (XXII), b0.3 124-7°. XXII (11.3 g.) similarly treated with p-aniaylmagneaium bromide gave p-aniayl 3-(N-isopropylnortropanyl)methyl ketone (XXIII), b0.2 160-4° and crystd. as a white solid. XXIII (7.5 g.) similarly treated with PhLi at 0° gave 1-(p-anisyl)-1-phenyl-3-(N-isopropylnortropane)ethanol (XXIV), white solid. Dehydration of XXIV with oxalic acid and H2O gave the ethylene, which when hydrogenated as deacribed above gave 1-p-anisyl-1-phenyl-2-(3-(N-isopropylnortropanyl)]ethane; methobromide salt. VIII (164 g.) in 500 ml. Et2O refluxed 3 hrs. with 30 g. LiAlH4 in 2 l. Et2O gave 3-tropanaethanol (XXV), m. 63-4° (C6H6-ligroins). XXV (10 g.) in 50 ml. CHCl3 treated with 14.3 g. SOCl2, refluxed 45 min., and isolation gave 1-chloro-2-(3-tropanyl)ethane-HCl, m. 167-8° (alc.-Et2O); free base, b0.9 81°. The base (47 g.) and 0.1 g. NaI refluxed 17 hrs. with 49 g. KCN in 175 ml. alc. and 75 ml. H2O, NaOH added to the residual mixt., and the product isolated gave 3-tropanepropionitrile (XXVI), b0.3 114-16°, n25D 1.4958. XXVI (25 g.) in 100 ml. 37% HCl refluxed several hrs., and evapd., the residue disaolved in 300 ml. alc., 5 ml. concd. H2SO4 added, and the residue treated with 40% NaOH gave Et 3-tropanepropionate (XXVII), b0.4 97-100°, n25D 1.4770. Similarly XXVII treated with PhLi gave 1,1-diphenyl-3-tropanepropanol (XXVIII), m. 141-2.5°. Dehydration of XXVII with concd. HCl and 40% NaOH added gave 1,1-diphenyl-3-(3-tropanyl)-1-propene (XXIX), b0.4 170-3°, m. 59-60°. XXIX (4.7 g.) hydrogenated over 5 g. Raney Ni gave 1,1-diphenyl-3-(3-tropanyl)propane as an oil; citrate, m. 170°; methobromide, m. 277°. XXVII reduced with 3 g. LiAlH4 gave 3-tropanepropanol (XXX), b2 128-31°. XXX (7.7 g.) treated with 10 g. SOCl2 gave the HCl salt, which treated with K2CO3 liberated 1-chloro-3-(3-tropanyl)propane (XXXI), b1 100-2°. XXXI (5 g.) refluxed 18 hrs. with 0.1 g. NaI, 5 g. KCN, 18 ml. alc., and 8 ml. H2O gave 3-tropanabutyronitrile (XXXII), b0.3 132-5°. XXXII (3 g.) refluxed several hrs. with concd. HCl and the product treated with 40% NaOH gave Et 3-tropanebutyrate (XXXIII), b0.5 115-19°. XXXIII (2.3 g.) similarly treated with p-tolyl magnesium bromide gave p-tolyl γ-(3-tropanyl)propyl ketone (XXXIV), b0.2 188-92°. XXXIV (1.5 g.) in 15 ml. Et2O treated with BuLi and 2-bromopyridine in Et2O gave 1-(2-pyridyl)-1-p-tolyl-3-tropanebutanol (XXXV), cryst. solid. XXXV (0.5 g.) dehydrated with 85% H2SO4, and the product reduced as described above gave 1-(2-pyridyl)-1-p-tolyl-4-(3-tropanyl)butane. II (9.2 g.) with MeLi gave dimethyl-3-tropanecarbinol, which was dehydrated by refluxing with AcOH and concd. HCl, and the product hydrogenated over Raney Ni to give 3-isopropyltropane as an oil. XXII (11.3 g.) treated with C6H13Li gave 1,1-dihexyl-3-(N-isopropylnortropane)ethanol (XXXVI), white solid. XXXVI (8 g.) refluxed 45 min. with AcOH and HCl gave an unsatd. product as the HCl salt which was hydrogenated over Raney Ni to 2-hexyl-1-[3-(N-isopropylnortropanyl)]octane as an oil. XXXIII (14.3 g.) similarly treated with cyclopentylmagnesium bromide gave cyclopentyl 3-(3-tropanyl)propyl ketone (XXXVII), b0.9 152-6°. XXXVII (3.5 g.) dehydrated and the product reduced over Raney Ni gave 1-cyclopentyl-1-phenyl-4-(3-tropanyl)butane, a colorless oil.

ACCESSION NUMBER: 1958:93020 CAPLUS
DOCUMENT NUMBER: 52:93020
ORIGINAL REFERENCE NO.: 52:16399b-i,16400a-i,16401a
TITLE: 8-Alkylnortropane derivatives
INVENTOR(S): Zirkle, Charles L.
PATENT ASSIGNEE(S): Smith, Kline & French Laboratories
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2800478		19570723	US 1955-519646	19550701

IT 112717-86-9 113222-63-2 114863-60-4
119016-27-2 119148-74-2 124119-19-3
(Derived from data in tha 6th Collective Formula Index (1957-1961))
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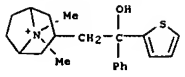
CN 3-(β-Hydroxy-β-2-thienylphenethyl)-8-methyltropanium bromide (6CI) (CA INDEX NAME)



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RN 113222-63-2 CAPLUS
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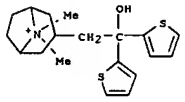

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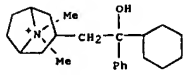

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RN 119016-27-2 CAPLUS
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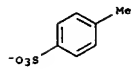

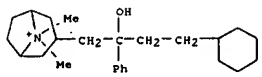

● Br⁻

RN 119148-74-2 CAPLUS
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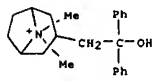

● Br⁻

RN 124119-19-3 CAPLUS
CN 3-(2-Hydroxy-2,2-diphenylethyl)-8-methyltropanium p-toluenesulfonate (6CI) (CA INDEX NAME)

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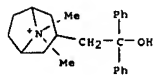
CRN 124119-18-2
CMF C23 H30 N O



CM 2

CRN 16722-51-3
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FULL ESTIMATED COST                                    53.81     229.51

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -5.46      -5.46

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 17:43:33 ON 28 NOV 2007
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